Charge Discreteness in Extended Quantum Circuits

H. Torres-Silva[1], D. Torres Cabezas[2]
[1]*Escuela de Ingeniería Eléctrica y Electrónica, Universidad de Tarapacá, Arica, Casilla 6-D, Chile E-mail: htorres@uta.cl*
[2]*Departamento Tecnologías de Información. Dirección del Trabajo, Agustinas 1253, Of. 509. Santiago, Chile. E-mail: torresdc@hotmail.com*

Abstract: A numerical wavefront solution for quantum transmission lines with charge discreteness is proposed for the first time. The nonlinearity of the system becomes deeply related to charge discreteness. The wavefront velocity is found to depend on the normalized (pseudo) flux variable. Finally we find the dispersion relation for the normalized flux ϕ / ϕ_0 .

I. Introduction

Currently nanostructures are embedded in countless devices and systems [1-5] . Naturally, at this scale and for low temperature, quantum mechanics plays a key role. Lately, much effort has been dedicated to study nanostructures, using as model of quantum circuits with charge discreteness [6-12]. In this article, we are interested in spatially transmission lines with charge discreteness. In this work we will consider a wavefront solution for an extended quantum circuit (transmission line). A sequence of bands and gaps is founded and characterized for this specific system with charge discreteness, which can extended for the description of more complex extended systems as dual transmission lines.. In section 2 we will introduce a generalization of classical transmission line. In section 3 we present the quantum transmission lines with charge discreteness, the Hamiltonian for coupled circuits, and the equations of motion for the spatially continuous system. In Sec. 4, the wavefront solution is considered. Finally, we give our conclusions.

II. Generalization of classical transmission line

Consider a homogeneous classical transmission line, assumed infinite, where the every cell is constituted of a LC circuit with inductance L and capacitance C. Assume that the interaction between neighbor cells is trough the capacitors (direct line), the classical evolution equations for the electrical current and charge, become in this case

$$L\frac{d}{dt}I_m = \frac{1}{C}(2q_m - q_{m+1} - q_{m-1}) \qquad (1)$$

Where the integer m designates the cell at position in the chain and, as usual, $I_m = \frac{d}{dt}q_m$ is the electrical current. The above linear equation of evolution becomes directly from the classical Lagrangian L_{ag} given by

$$L_{ag} = \sum_m (\frac{L}{2}I_m^2 - \frac{1}{2C}(q_m - q_{m-1})^2) \qquad (2)$$

Using the Lagrange equations one obtains (1).
From the usual definition for the conjugate variables, in this case the magnetic flux

$$\frac{\partial}{\partial I_m}L_{ag} \qquad (3)$$

And the expression for the Hamiltonian in terms of these variables it becomes

$$H = \sum_m (\frac{1}{2L}\phi_m^2 + \frac{1}{2C}(q_m - q_{m-1})^2) \qquad (4)$$

To solve the coupled systems (1) is direct since it corresponds to the second order discrete wave equations,

$$L\frac{d^2}{dt^2}q_m = \frac{1}{C}(-2q_m + q_{m+1} + q_{m-1}) \qquad (5)$$

Supporting solutions like a plane wave. Explicitly,

$$q_m = q_0 \exp(i\omega t - ikm) \quad (6)$$

Where, as usual in these cases , the frequency ω and the wavenumber k become related through the dispersion relation.

The variable q_0 is a constant parameter describing the amplitude of the wave. Note that we have considered by sake of simplicity the lattice-size a as one. That is the adimensional number k in the equation (6) is really ka .

After some algebra, one obtains from (5) the dispersion relation

$$\omega^2 = \frac{4}{LC}\sin^2(\frac{k}{2}) \quad (7)$$

Here we have:

a) The infrared limit ($ka \to 0$) related to the continous –space structure becomes direct and corresponds to the dispersion relation $\omega = k/\sqrt{LC}$, namely a non dispersive medium.

b) Equation (7) defines a system with only a band structure

c) The quantization of this transmission line is direct since it is analogue to the case of mechanical vibration of a homogeneous system. The Hamiltonian is

$$\hat{H} = \sum_k \frac{2}{\sqrt{LC}}\left|\sin(\frac{k}{2})\right|(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2}) \quad (8)$$

With the usual creation-destruction operators of the mode k.

From a general point of view, for arbitrary composition od a cell in the line, the Hamiltonian of this generalized electrical transmission line becomes quadratic, namely,

$$H = \sum_{m,s}(\frac{1}{2}(\frac{1}{L})_{m,s}\phi_m\phi_s + \frac{1}{2}(\frac{1}{C})_{m,s}q_m q_s) \quad (9)$$

Quantization is carried-out here in the standard way. For homogeneous systems where

$$(\frac{1}{L})_{m,s} = (\frac{1}{L})_{m-s} \quad (10)$$

And

$$(\frac{1}{C})_{m,s} = (\frac{1}{C})_{m-s} \quad (11)$$

Is always possible to transform the hamiltonian to normal modes. That is, using the Fourier transform to separate variables we have

$$H = \sum_k H_k \quad (12)$$

corresponding to an ensemble of harmonic oscillators.

III. Quantum transmission lines with charge s discreteness

As illustration and following [8, 9, 13], and from the Hamiltonian (4), the usual quantization procedure for flux and charge, and the prescription (2) for charge discreteness, we could construct the quantum Hamiltonian for the direct line with charge discreteness (q_e), the Hamiltonian may be written as:

$$\hat{H} = \sum_{m=-\infty}^{\infty}\left\{\frac{2\hbar^2}{Lq_e^2}\sin^2\frac{q_e}{2\hbar}\hat{\phi}_m + \frac{1}{2C}(\hat{Q}_m - \hat{Q}_{m-1})^2\right\} \quad (13)$$

Where the index m describes the cell (circuit) at position m, containing an inductance L and capacitance C. The conjugate operators, charge $\hat{Q}$ and pseudoflux $\hat{\phi}$, satisfy the usual commutation rule

$$\left[\hat{Q}_m, \hat{\phi}_{m'}\right] = i\hbar\delta_{m,m'} \text{ and } \left[\hat{Q}_m, \hat{Q}_s\right] = \left[\hat{\phi}_m, \hat{\phi}_s\right] = 0 . \quad (14)$$

A spatially extended solution of Eq. (1) corresponds to the quantization of the classical electric transmission line with discrete charge (i.e. elementary charge q_e). Note that in the formal limit $q_e \to 0$ the

above Hamiltonian gives the well-known dynamics related to the one-band quantum transmission line, similar to the phonon case. The system described by Eq. (1) is very cumbersome since the equations of motion for the

operators are highly nonlinear due to charge discreteness. However, this system is invariant under the transformation $\hat{Q}_k \to \hat{Q}_k + \alpha$, that is, the total pseudoflux operator $\hat{\phi} = \sum \hat{\phi}_m$ commutes with the Hamiltonian; in turn, the use of this symmetry helps us in simplifying the study of this system. To handle the above Hamiltonian, we will assume a continuous approximation (infrared limit); that is we use $Q_m - Q_{m-1} \approx \partial Q / \partial x$. In this way, it is possible to re-write the sum of Eq. (1) as the integral $\sum_{m=-\infty}^{\infty} \approx \int_{-\infty}^{\infty} dx$, where x is a dimensionless variable used to denote the position in the chain (i.e. the equivalent of k), since we have not introduced so far the cell size of the circuit. In this approximation, the Hamiltonian (13) becomes

$$\hat{H} = \int \hat{H}_m dx = \int \left(\frac{2\hbar^2}{Lq_e^2} \sin^2 \frac{q_e}{2\hbar} \hat{\phi}_m - \frac{1}{2C} \left(\frac{\partial Q}{\partial x}\right)^2\right) dx \tag{15}$$

where $\hat{H}_m$ represents the Hamiltonian density operator for the fields. From the above Hamiltonian we find the equations of motion (Heisenberg equations) for the field operators:

$$\frac{\partial}{\partial t} \hat{\phi} = \frac{1}{C} \frac{\partial^2}{\partial x^2} \hat{Q} \tag{16}$$

$$\frac{\partial}{\partial t} \hat{Q} = \frac{\hbar}{Lq_e} \sin\left(\frac{q_e}{\hbar}\right) \hat{\phi} \tag{17}$$

Note that, in circuit with discrete charge the electric current (17) is bounded and periodic in the pseudo flux. The nonlinearity in the electrical current evolution equation makes the problem very difficult.
An independent or closed equation for the pseudo flux is easily obtained as

$$\frac{\partial^2}{\partial t^2} \hat{\phi} = \frac{1}{LC} \frac{\hbar}{q_e} \frac{\partial^2}{\partial x^2} \left\{ \sin\left(\frac{q_e}{\hbar} \hat{\phi}\right) \right\} \hat{\phi} \tag{18}$$

Here, we consider a cell of size **a** and the limit where the spatial variations of the dynamic variables is longer than a. In this case defining the capacitance C (per unit of length), the inductance L (per unit of length), the length x is $x = ma$, and keeping the limit $a \to 0$.

IV. Wave front solutions

We proceed in the standard way, by assuming travelling wave solutions for our operators, and the semi classical Hamiltonian is:

$$\hat{H} = \int \hat{H}_m dx = \int \left(\frac{2\hbar^2}{Lq_e^2} \sin^2 \frac{q_e}{2\hbar} \hat{\phi}_m - \frac{1}{2C} \left(\frac{\partial Q}{\partial x}\right)^2\right) dx \tag{19}$$

Equation (19) corresponds to an eigenvalue problem for the non-linear super operator $\sin \hat{\phi}$

$$\hat{H} = \int \hat{H}_m dx = \int \left(\frac{2\hbar^2}{Lq_e^2} \sin^2 \frac{q_e}{2\hbar} \hat{\phi}_m - \frac{1}{2C} \left(\frac{\partial Q}{\partial x}\right)^2\right) dx,$$

The equations of motion (Heisenberg equations) are

$$\frac{\partial \phi}{\partial t} = \frac{\partial H}{\partial Q} - \frac{\partial}{\partial x} \frac{\partial H}{\partial Q_x}, \quad Q_x = \frac{\partial Q}{\partial x}, \quad \frac{\partial Q}{\partial t} = \frac{\partial H}{\partial \phi}$$

Performing the appropriate calculations we obtain

$$\frac{\partial \phi}{\partial t} = \frac{1}{C} \frac{\partial^2 Q}{\partial x^2} \tag{20}$$

And

$$\frac{\partial Q}{\partial t} = \frac{\hbar}{Lq_e} \sin\left(\frac{q_e}{\hbar}\right) \phi \tag{21}$$

Note that the formal limit $q_e \to 0$ gives us the usual linear wave equation for transmission line in electric networks.
let

$$\phi \to \phi e^{ikx}, \; Q \to Qe^{ikx} \;, \; \phi_0 = \frac{\hbar}{q_e} \tag{22}$$

Then the wavefront equations are

$$\frac{1}{\phi_0}\frac{\partial^2 \phi}{\partial t^2} = -\frac{k^2}{LC}\sin(\phi/\phi_0) \tag{23}$$

And

$$\frac{1}{Q}\frac{\partial^2 Q}{\partial t^2} = -\frac{k^2}{LC}\cos(\phi/\phi_0) \tag{24}$$

And dispersión relation is obtained from:

$$\omega^2 \frac{\phi}{\phi_0} = \frac{k^2}{LC}\sin(\phi/\phi_0) \text{ and } \omega^2 \frac{Q}{Q_0} = \frac{k^2}{LC}\cos(\phi/\phi_0) \tag{25}$$

$$\omega^4(1+(\phi/\phi_0)^2) = \frac{k^4}{(LC)^2}$$

$$v^2 = \frac{\omega^2}{k^2} = \frac{1}{LC}\frac{1}{(1+(\phi/\phi_0)^2)^{1/2}}$$

$$v^2 LC = \frac{1}{(1+(\phi/\phi_0)^2)^{1/2}} \tag{26}$$

which in the limit $q_e \to 0$ becomes the usual one band transmission wave equation.

$$v^2 = \frac{\omega^2}{k^2} = \frac{1}{LC}$$

Equation (26) is plotted for short quantum circuits,here, we show the figure 1, where, $0 < \phi/\phi_0 < 1$

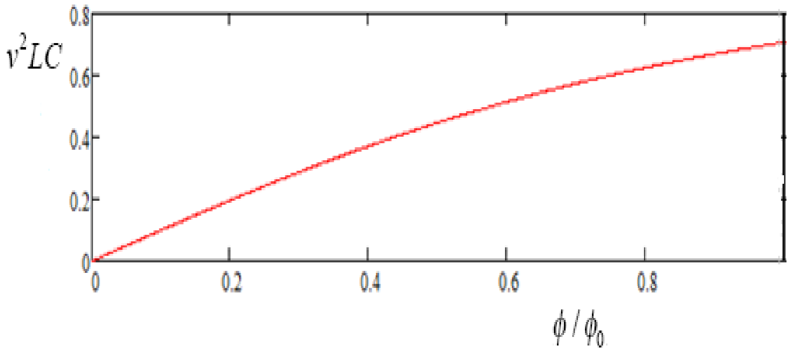

Figure 1. Plot of the velocity of the wavefront as a function of the flux parameter. Here, there is a structure of bands and gaps $0 < \phi/\phi_0 < 1$, $v^2 LC = 0$ if $\phi/\phi_0 \neq 0.1, 0.2, 0.3.....$ 1.0. This structure is a direct consequence of charge discreteness, an effect that disappears when $q_e \to 0$.

Figure 2, show s the dispersion relation for $1 < \phi/\phi_0 < \infty$, $x = \phi/\phi_0$ .Here the quantum transmission line present structure of bands and gaps where real solutions appear when $v^2 LC > 0$ as it is shown in table 1.

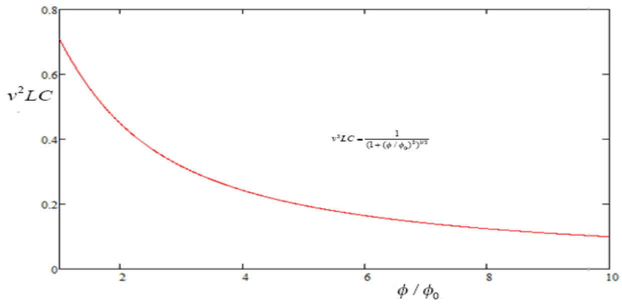

Figure 2. Plot of the velocity of the wavefront as a function of the flux parameter.

Here also we have a structure of bands and gaps. $1 < \phi/\phi_0 < \infty$. When ϕ/ϕ >>1, wave velocity goes to zero.

Table1.

n	x	v^2LC
1	4.4896	<0
2	7.7245	>0
3	10.9038	<0
4	14.0660	>0
5	17.2206	<0
6	20.3712	>0
7	23.5194	<0
8	26.6660	>0
9	29.8115	<0
10	32.9563	>0

Tabla 1 is obtained from equations (25) which can be put as $x = \sin x / \cos x$ and n is a number that appears in the approximated solution of $x = \sin x / \cos x$ [14].

$$x = \exp(\cosh^{-1}(2n+1)\pi/4)) \qquad (27)$$

The numerical results of table 1, may be useful to estimate thermal properties of a quantum LC circuit with charge discreteness [15].

V. Conclusions

For the quantum electric transmission line with charge discreteness described by the Hamiltonian (13), and equations of motion (16-17), wavefront solution was found. One condition on the velocity generates a band-gap structure dependent on the pseudo flux parameter (see figure 1), namely, there exist regions (values of ϕ/ϕ_0) for which a solitary wavefront propagates with constant speed according the value of ϕ/ϕ_0. The main results of this work are the existence of the band-gap structures for $0 < \phi/\phi_0 < 1$ and for $\infty < \phi/\phi_0 < 1$.

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